U.S. DEPARTMENT OF ENERGY | Nuclear Energy

An Overview of NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Fiscal Year 2017 Annual Planning Webinar

Advanced Modeling & Simulation Office (NE-41)
Office of Science and Technology Innovation (NE-4)
U.S. Department of Energy

August 2016

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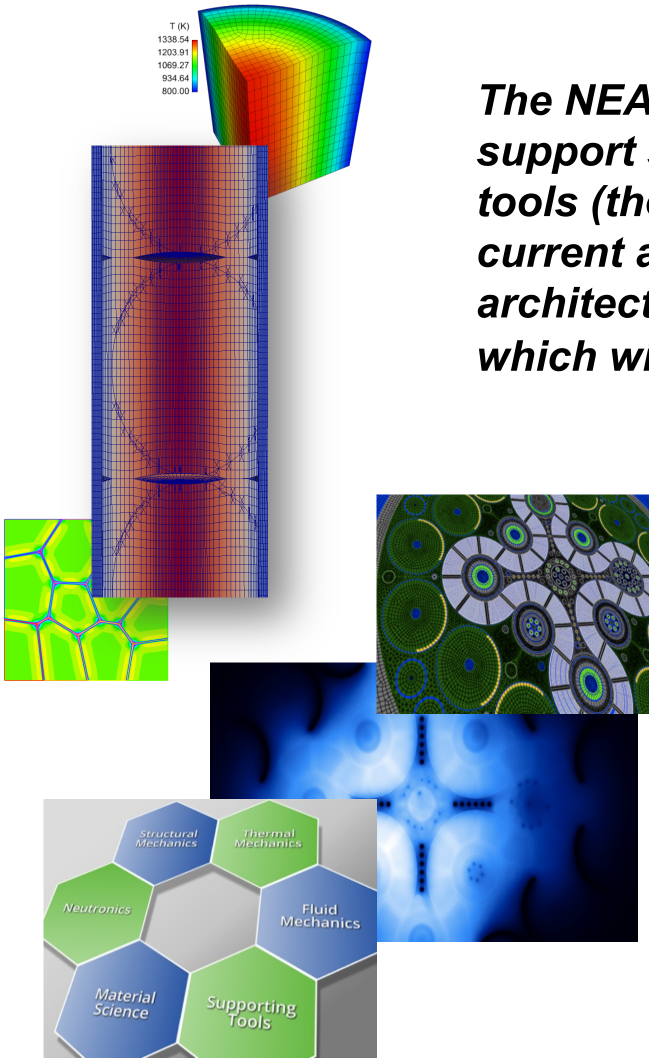
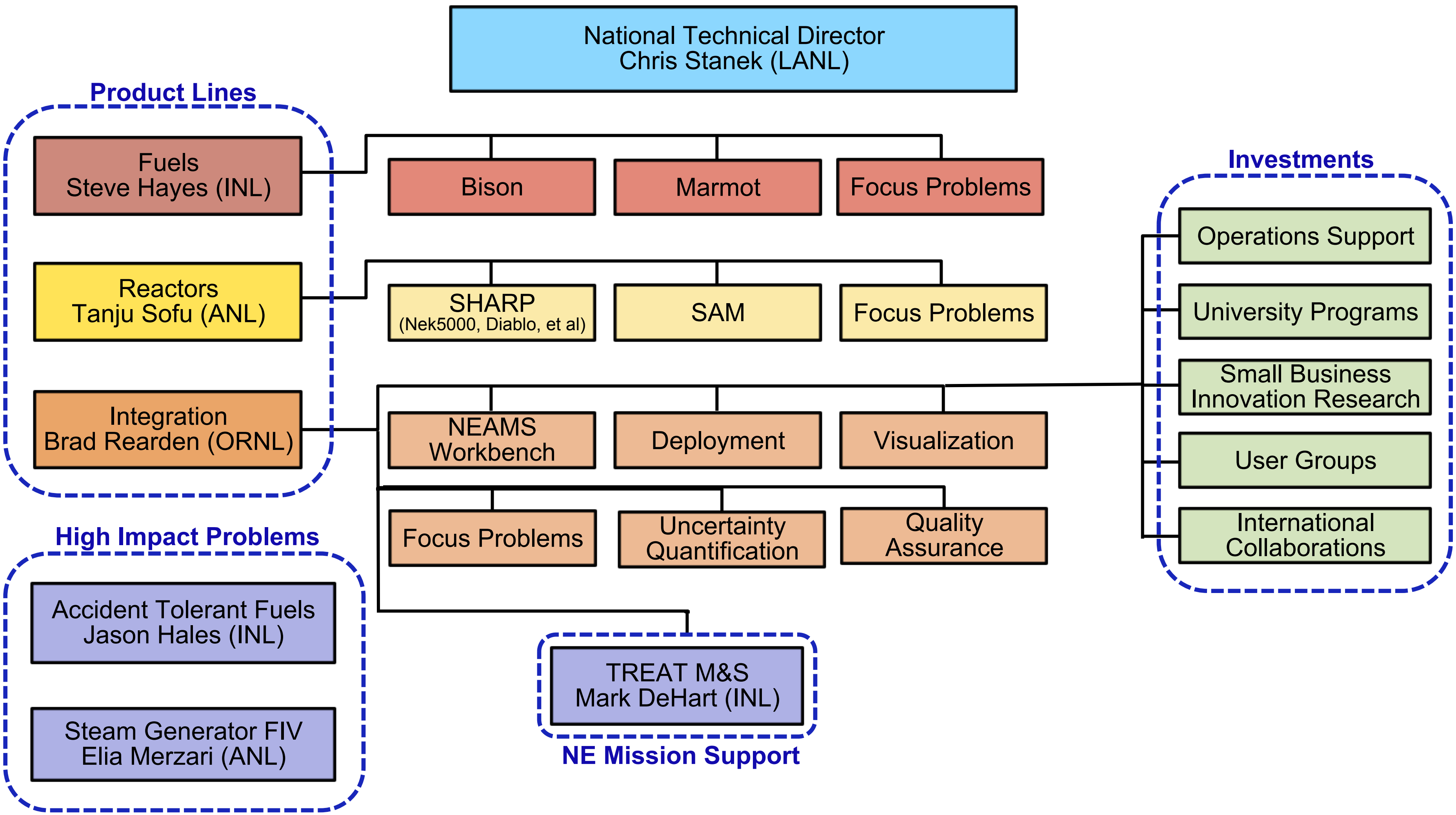
Nuclear Energy Advanced Modeling and Simulation (NEAMS)



The NEAMS Value Proposition: Develop, apply, deploy, and support state-of-the-art predictive modeling and simulation tools (the NEAMS ToolKit) for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities, which will –

- **Enable transformative scientific discovery and insights otherwise not attainable or affordable**
- **Accelerate both the solutions to existing problems as well as the deployment of new designs, for current and future (advanced) reactors**
- **Solve problems identified as significant by industry, and consequently expand validation, application, and long-term utility of these advanced tools**

NEAMS Mission Areas



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NEAMS Organizational Structure

Leadership Council

National Technical Director
Chris Stanek (LANL)

ATF HIP
Jason Hales (INL)

Fuels Product Line
Steve Hayes (INL)

Integration Product Line
Brad Rearden (ORNL)

Reactors Product Line
Tanju Sofu (ANL)

SGFIV HIP
Elia Merzari (ANL)

Dan Funk
Advanced Modeling & Simulation Office (NE-41)

Shane Johnson
Deputy Assistant Secretary, Office of Science and Technology Innovation (NE-4)

Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

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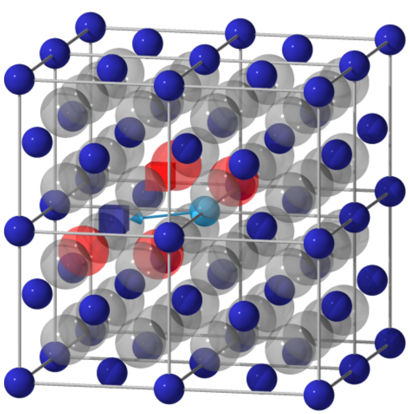
FPL

NEAMS - Fuels Product Line (FPL)

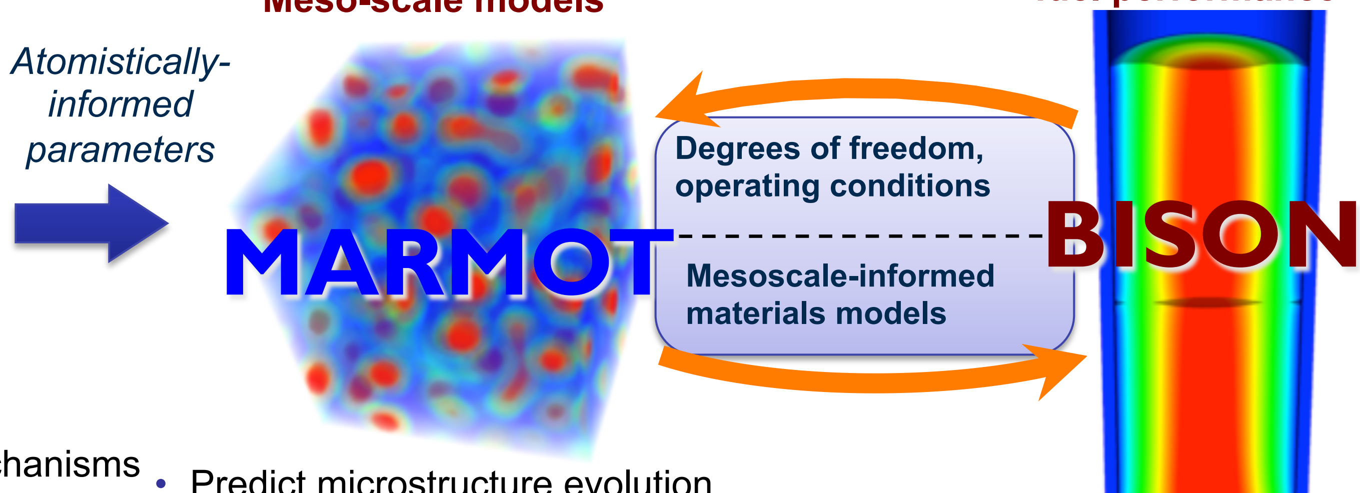
- **Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds**
- **<u>Goal</u>: Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling - applied to existing, advanced (including accident tolerant) and used fuel.**

Atomistic simulations



Meso-scale models

Engineering scale fuel performance



- Identify important mechanisms
- Determine material parameter values

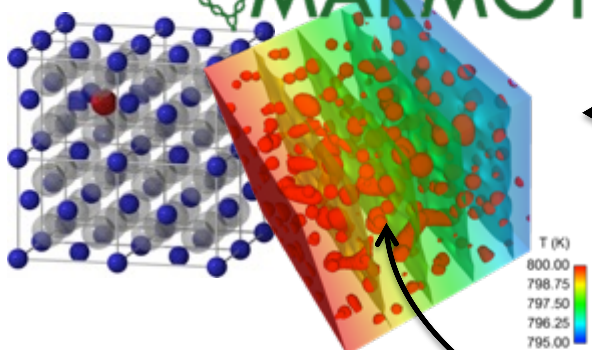
- Predict microstructure evolution
- Determine effect of evolution on material properties

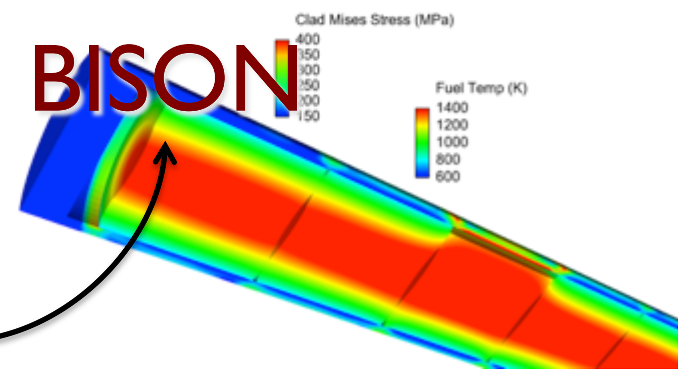
- Predict fuel performance and failure probability

FPL

NEAMS - MOOSE-BISON-MARMOT

MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability





Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

MOOSE
Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

R&D 100 2014 Winner

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FPL

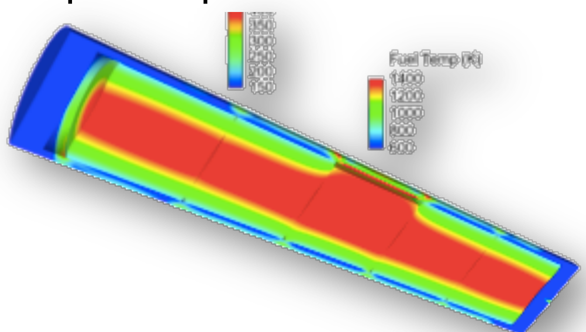
NEAMS – BISON Advanced Validation

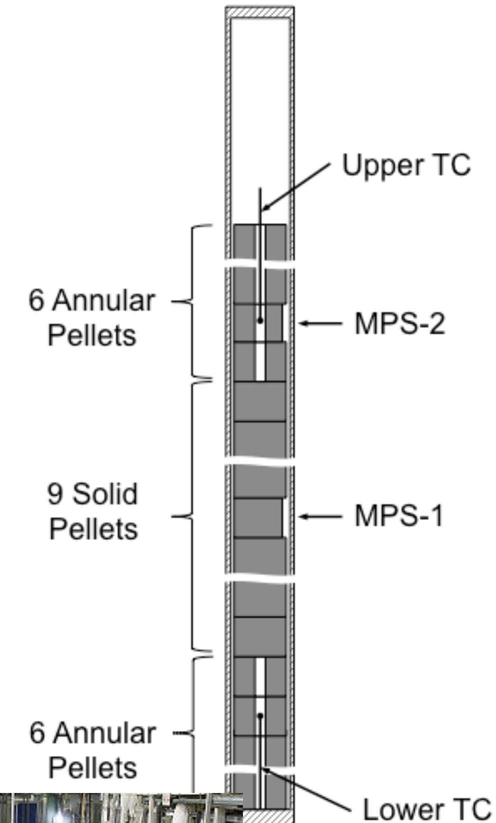
Halden Missing Pellet Surface Experiment

Manufacturing flaws (“missing pellet surface” defects) in fuel pellets have been root cause of fuel failures. Pellet-cladding interaction (PCI) is a CASL challenge problem.

Validation experiments being planned for the Halden reactor later this year.

Example of a 3D fuel performance code addressing a 3D applied problem – which requires specific validation





Once validated, further analysis using BISON to define an MPS geometry threshold could used to inform fuel manufacturing tolerances.

The OECD Halden Reactor Project

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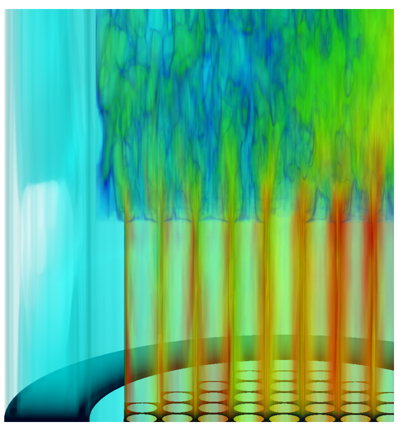
RPL

NEAMS - Reactors Product Line (RPL)

Develops and deploys high-fidelity, coupled-physics simulation capability for advanced reactors using the *Sharp* code suite, which consists of:

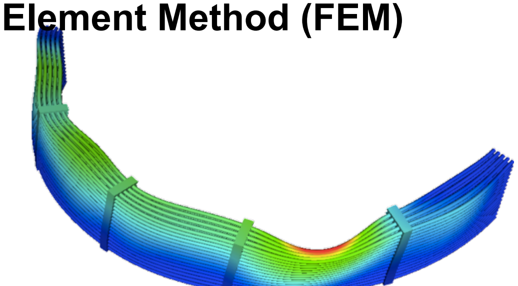
Nek5000 –Thermal-Hydraulics

Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics



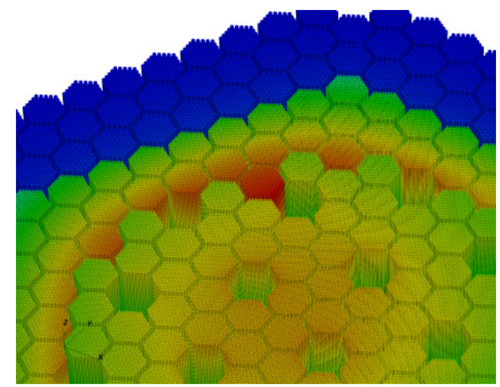
DIABLO – Structural Dynamics

3-D thermal-structural and thermal mechanics analysis using a time implicit Finite Element Method (FEM)



PROTEUS – Neutronics

Can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling

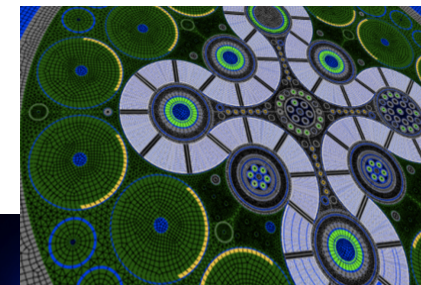


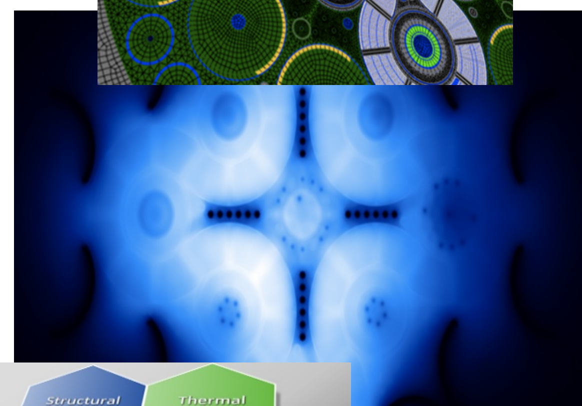
RPL

NEAMS - SHARP-3D

Coupled Multiphysics Simulations for Fast Reactors

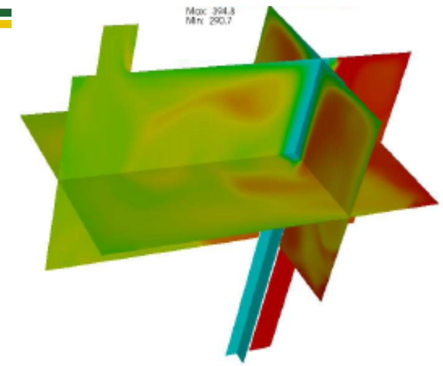
- **SHARP-3D (with modules, MC2-3, PROTEUS, Nek-5000, DIABLO) provide high-fidelity/multi-scale and multi-physics simulations of core dynamics, core mechanics, and core thermal-hydraulics over time scales from picoseconds to seconds to days, with coupling as needed**
  - Help researchers understand complex, coupled phenomena that are hard to model and measure
  - Support conceptual design of advanced reactors of all types
  - Simulate safety transients using high-fidelity, coupled neutronics, thermal-fluids, thermal-mechanics, and fuel models
  - Accurate solutions even with lower-fidelity models
  - Demonstrate advanced validation and uncertainty quantification approaches
  - Leverages leading-edge high performance computing capabilities

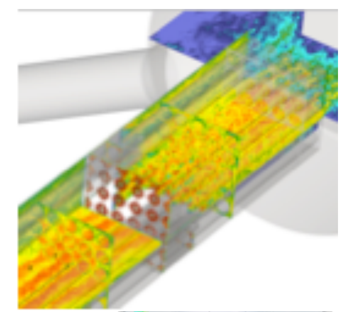


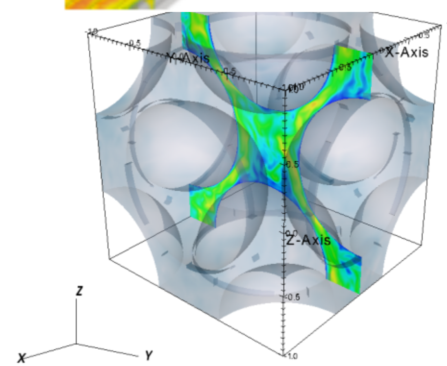


NEAMS - Nek5000
Thermal Hydraulics Module

- **Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics**
  - Computational Fluid Dynamics (CFD) toolset using the Spectral Element Method (SEM)
  - Supports conjugate heat transfer analysis
  - Includes Stability Analysis toolkit with adjoint and Proper Orthogonal Decomposition capabilities
- **Key Capabilities**
  - Unstructured grid
  - Incompressible and weakly compressible
  - DNS, LES and RANS formulations
  - Conjugate heat transfer
  - ALE formulation for moving meshes
- **Open Source – available for download at nek5000.mcs.anl.gov**
- **Demonstrated for up to 1,000,000 cpu processes and several billion geometric grid points.**
  - Also runs on desktop workstations



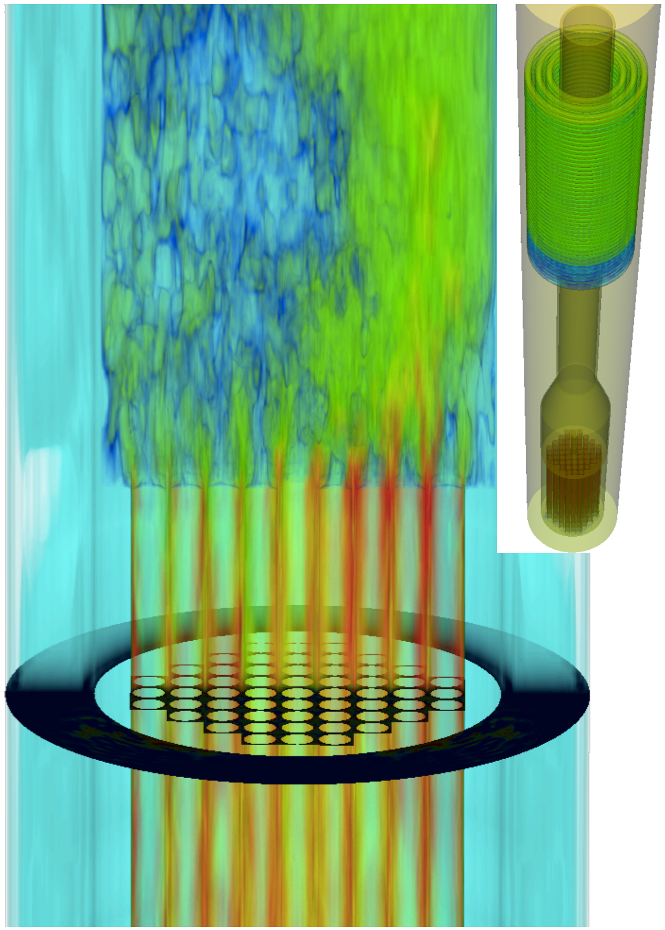




DNS: Direct Numerical Solution
LES: Large Eddy Simulation
RANS: Reynolds-Averaged Navier-Stokes
ALE: Arbitrary Lagrangian Eulerian.

RPL

NEAMS - Nek5000
MASLWR Experiment Simulation

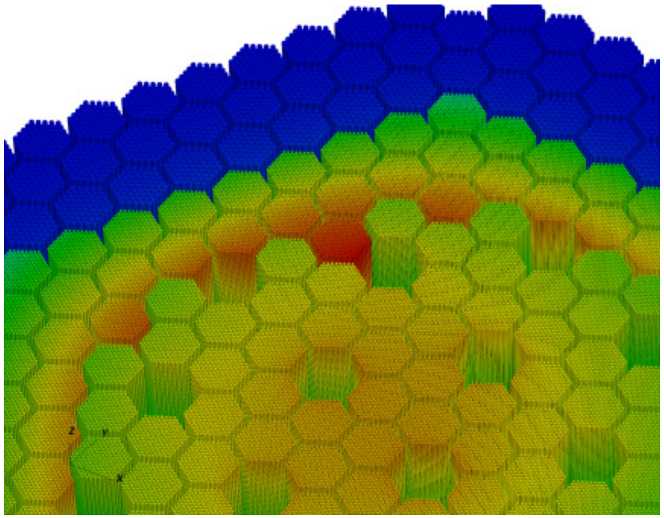


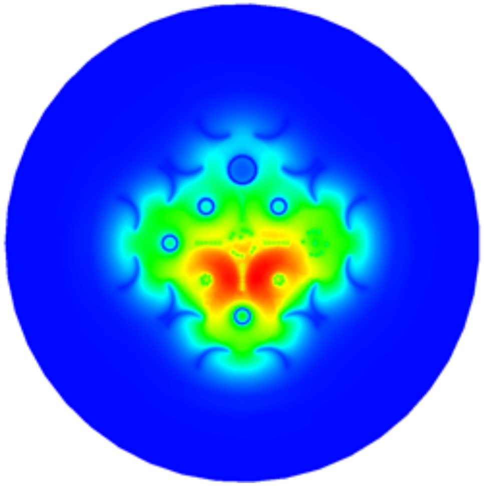
Instantaneous LES velocity

- MASLWR: Multi-Application Small Light Water Reactor Experiment
- Scaled system level facility to examine natural circulation phenomena important to small modular reactors (SMR)
- Natural convection as hot water exits the top of the core difficult to treat in many CFD codes
- Challenging problem to handle - Nek5000 being used for simulation

RPL

NEAMS - PROTEUS
Unstructured Grid Neutronics



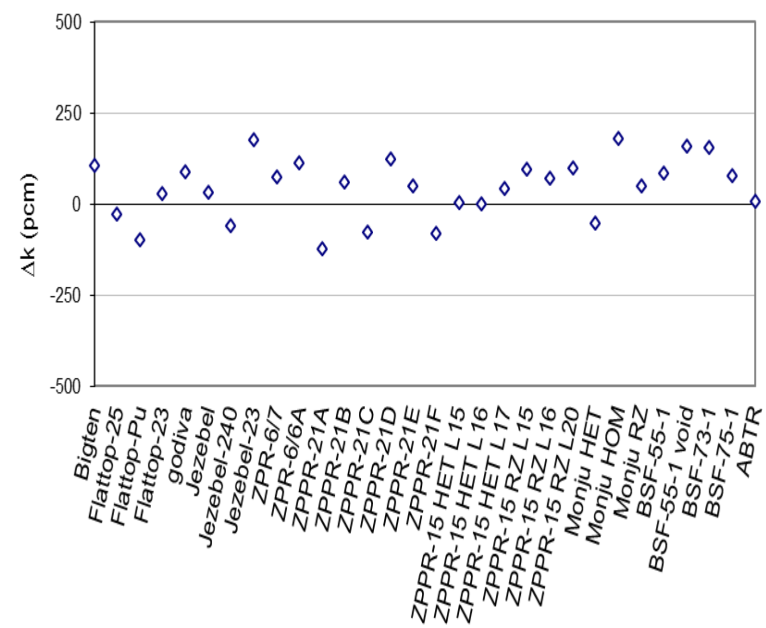


- **PROTEUS – the neutronics module**
  - Can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling
- **Multigroup cross sections generated with MC^2-3**
- **Integrated depletion with ORIGEN from SCALE**
- **Public release now available from ANL**
- **Successfully used on real problems- ATR, ZPR, MONJU, PHENIX, EBRII…**
- **Validated against ZPR experiment foil reaction rates and k-effective**
  - More needed!
- **Demonstrated scalability to more than 200,000 CPU cores and billions of degrees of freedom.**
  - Also runs on desktop workstations

RPL

NEAMS - MC²-3
Multigroup Cross Section Generation Code

- **Developed under the NEAMS program to generate fast reactor multigroup cross sections for conventional (DIF3D) and high-fidelity (PROTEUS) codes**
  - Improved resonance self-shielding using pointwise cross section integration (including analytic Doppler broadening) and improved modeling of the local heterogeneity effect based on 1D geometry
  - Accurate multigroup cross section accounting for the whole-core spectrum effect by coupling with TWODANT
- **V&V using many fast reactor benchmark problems and experiments**
- **Being used by the ART, as one of the major design codes, as well as many other users (TerraPower, KAERI, UNIST, many U.S. national labs and universities**



Comparison of Core Eigenvalues between MC²-3/DIF3D and MCNP

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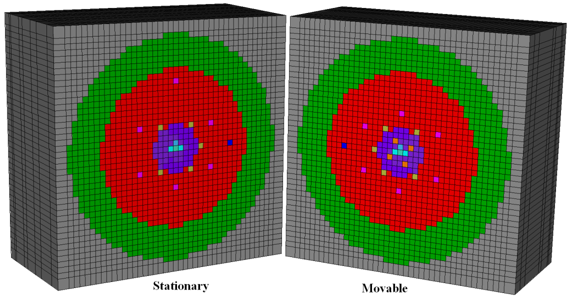
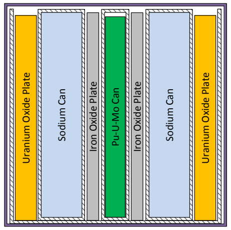
NEAMS - MC²-3

Current Status

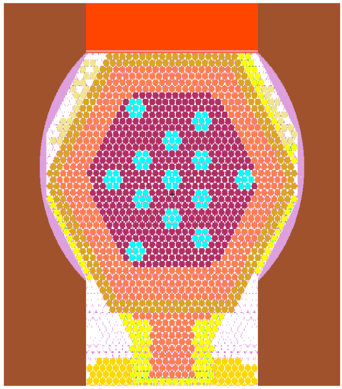
- **Recent Progress**
  - 3D MOC transport calculation capability to more accurately account for the heterogeneity effect of complex geometry problems
  - Thermal cross section capability which allows the code to be used for thermal reactor applications
  - Generation of ENDF/B-VII.1 cross section library
- **Needs in association with the new capabilities**
  - Performance improvements in terms of computation time and efficiency, solution stability, efficient coupling with PROTEUS, etc.
  - Significant efforts on V&V tests for the new capabilities
  - Further efforts on uncertainty evaluation



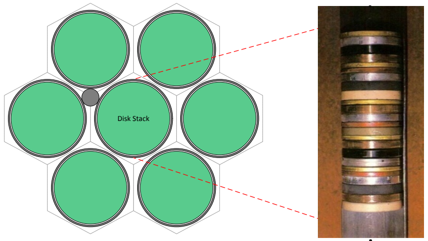
ZPPR



ZPPR Fuel



BFS

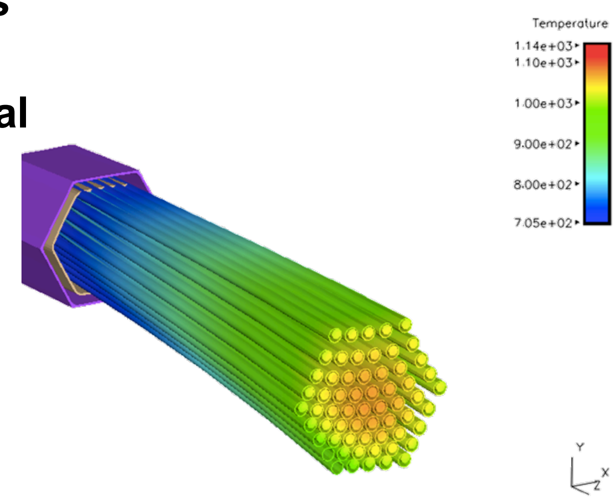


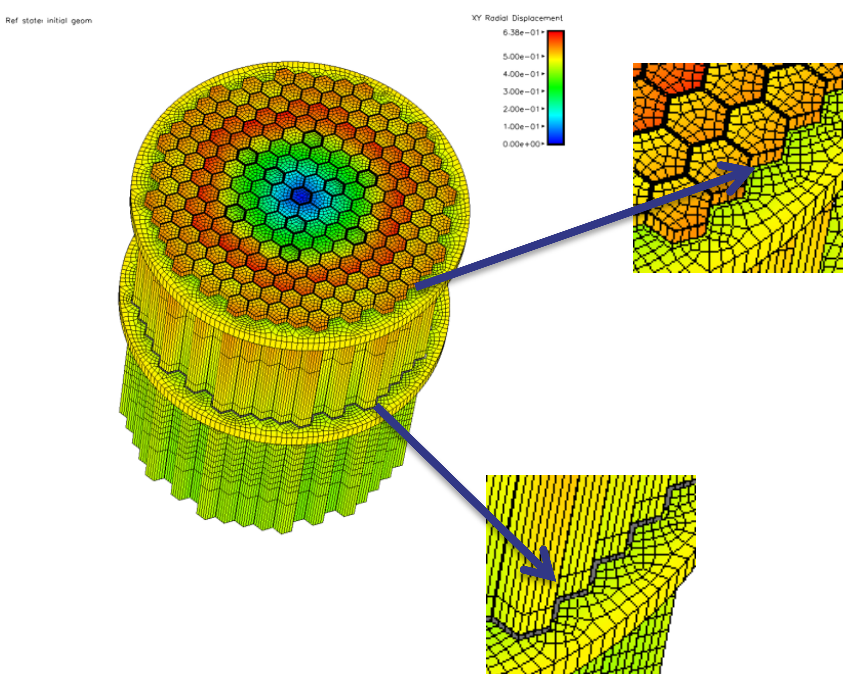
BFS Fuel

RPL

NEAMS – DIABLO
Structural Mechanics

- **3-D thermal-structural and thermal mechanics analysis using a time implicit Finite Element Method (FEM)**
- **Prediction of deformation and stresses under structural and thermal loads**
- **Includes a variety of contact modeling options**
- **Includes connectivity to selected soil-structure interaction models for seismic analysis**





- **Early user releases available, with updated user guides, methodology manuals, etc. in development**
- **Validated for a variety of standard structural mechanics benchmark**
  - Additional specific nuclear energy application validation needed
- **Demonstrated scalability to petascale computing platforms and large problems**
  - Also runs on desktop workstations

IPL

NEAMS - Integration Product Line (IPL)

- **NEAMS FPL and RPL provide many advanced tools, but they often require large computational resources, can be difficult to install, and require expert knowledge to operate.**
- **Goal: Integrate robust multiphysics capabilities and current production tools to provide ease-of-use and deployment to end users, enabling the use of high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems and experiments.**

- **Desired attributes:**
  - Convenient access to high-fidelity simulations to inform lower-order models
  - Common user interface
  - Simplified common input to many codes
  - Visualization
  - Uncertainty quantification
  - Quality assurance
  - Verification and validation
  - Application to design systems and recognized benchmarks

- **Leverage investments in:**
  - Nuclear Energy University Programs (NEUP)
  - Small Business Innovation Research (SBIR)
  - International collaborations
  - User groups
  - Operations support

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IPL

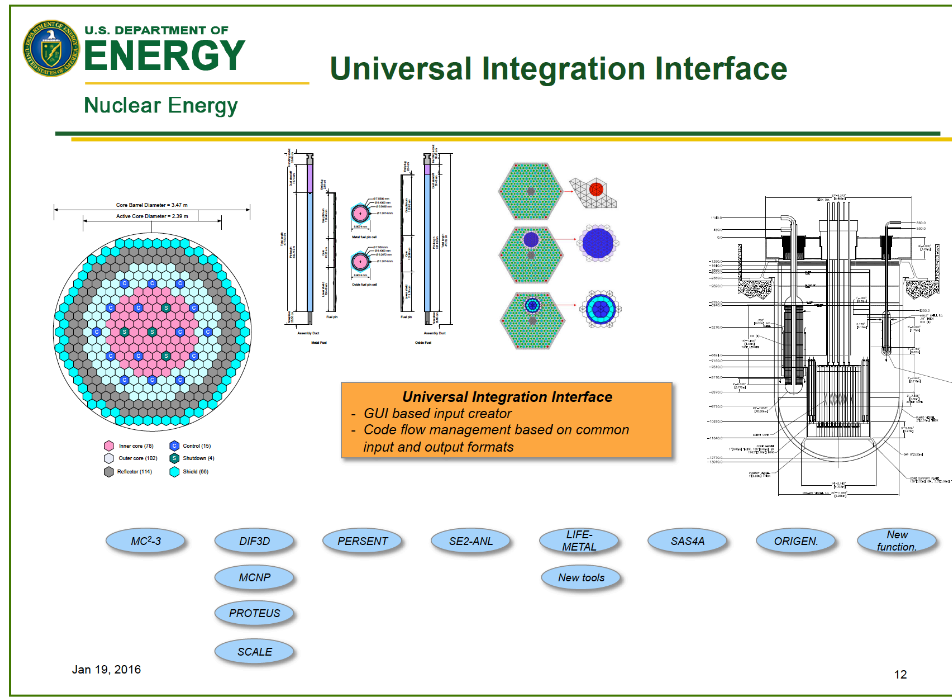
NEAMS - Integration Product Line (IPL)

NEAMS LC changes (IPL, RPL and NTD) and priority shift have resulted in refactored IPL

When defining 5 year goals and path to achieve them, emphasis placed upon: Proactive customer engagement to ensure relevance, *i.e. deployment.*

Specific near-term question:

•*How to provide technology of value to Advanced Reactor Technologies (ART) Program and the Nuclear Regulatory Commission (NRC)?*

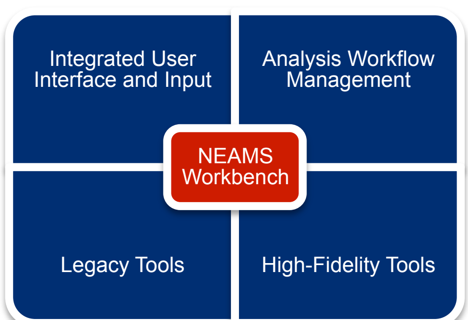


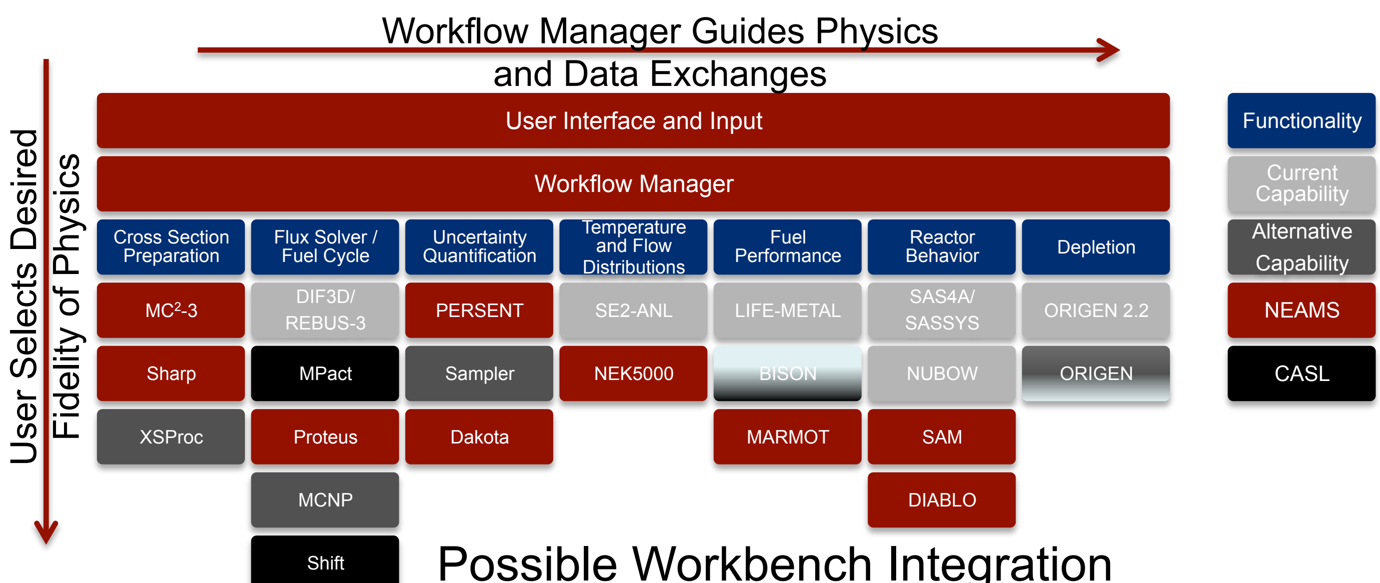
Dialogue with ART = "universal" interface
•Improved use of existing tools
•Gateway to modern tools
•Focus on consistency and ease-of-use
(Slide: T.K. Kim – ANL)

IPL

NEAMS – IPL/Workbench

- **Integrate current production tools with advanced tools under an integrated user interface and workflow manager**
- **Leverage modern user interface from SCALE, which is co-sponsored by NRC**
- **Leverage templating/input expansion engine from UNF-ST&DARDS and SCALE so that engineering parameters can be expanded to specific input for analysis with varying levels of fidelity in several codes**
- **Desire to integrate many tools for many types of systems**



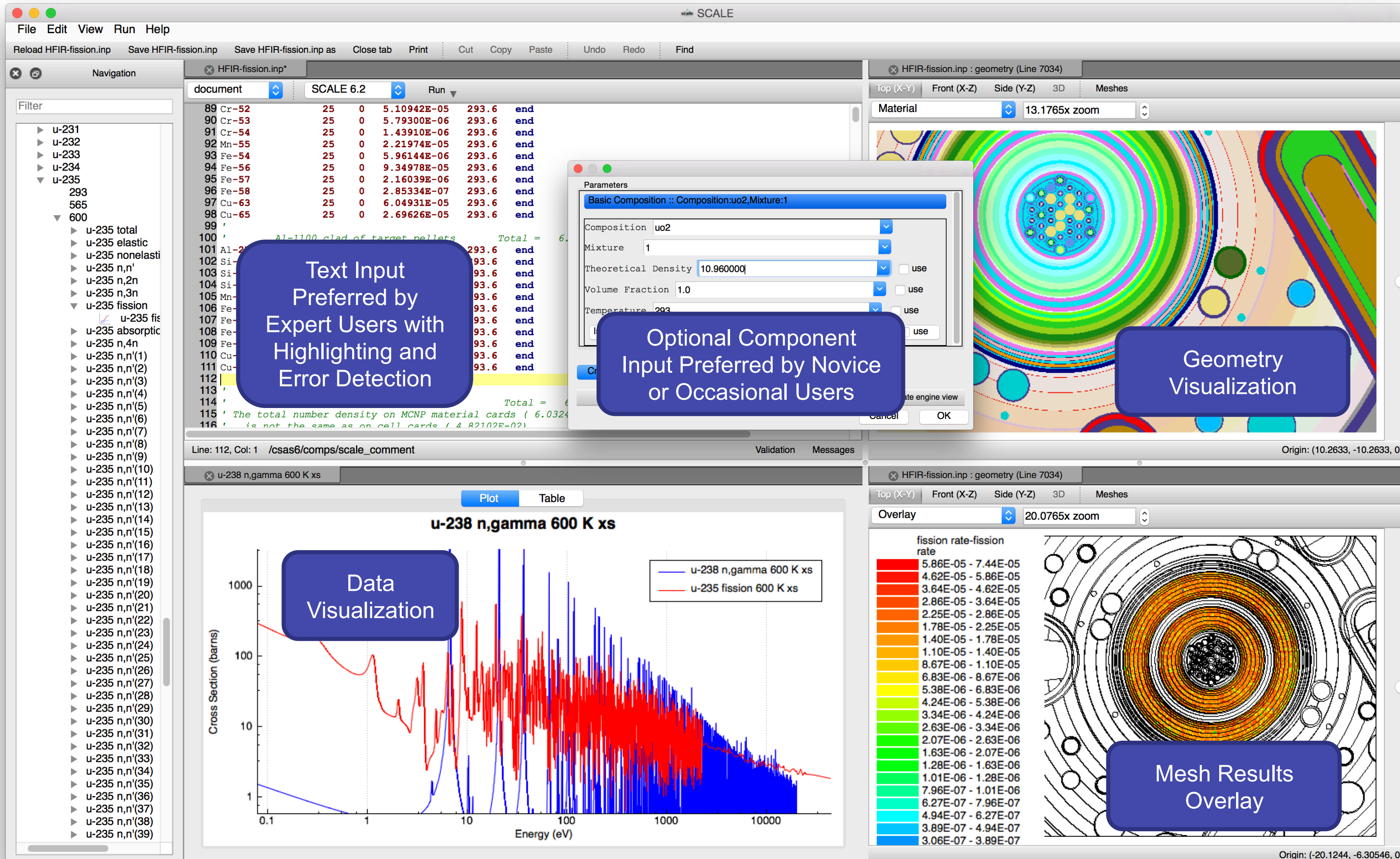


Possible Workbench Integration for Fast Reactor Analysis

IPL

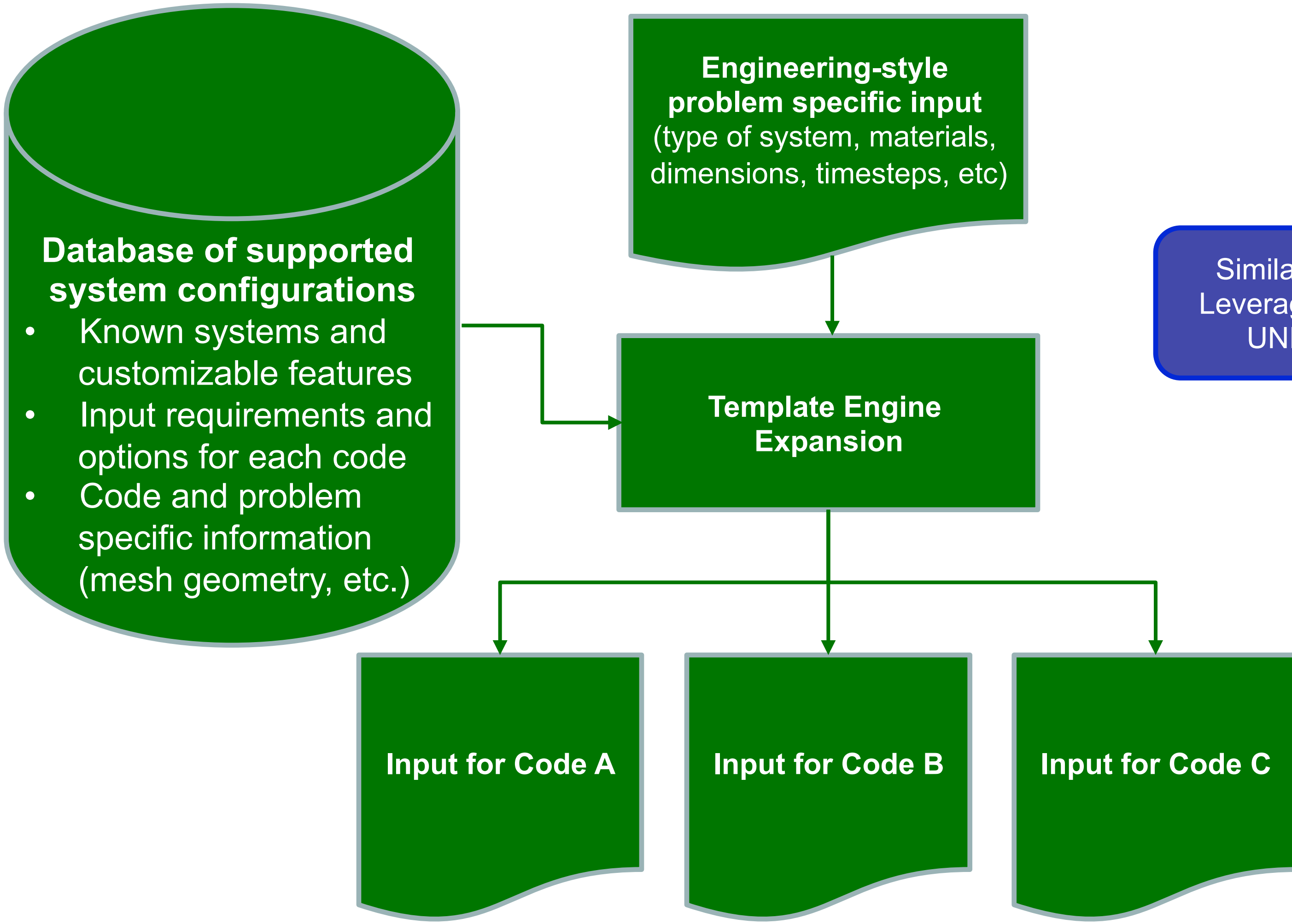
NEAMS – Workbench User Interface

Snapshot of Fulcrum (from SCALE)



NEAMS – IPL/Workbench

Templated Common Input for Many Codes with Varying Levels of Fidelity



Similar to CASL VERA-IN concept; Leverages Template Engine used for UNF-ST&DARDS and SCALE

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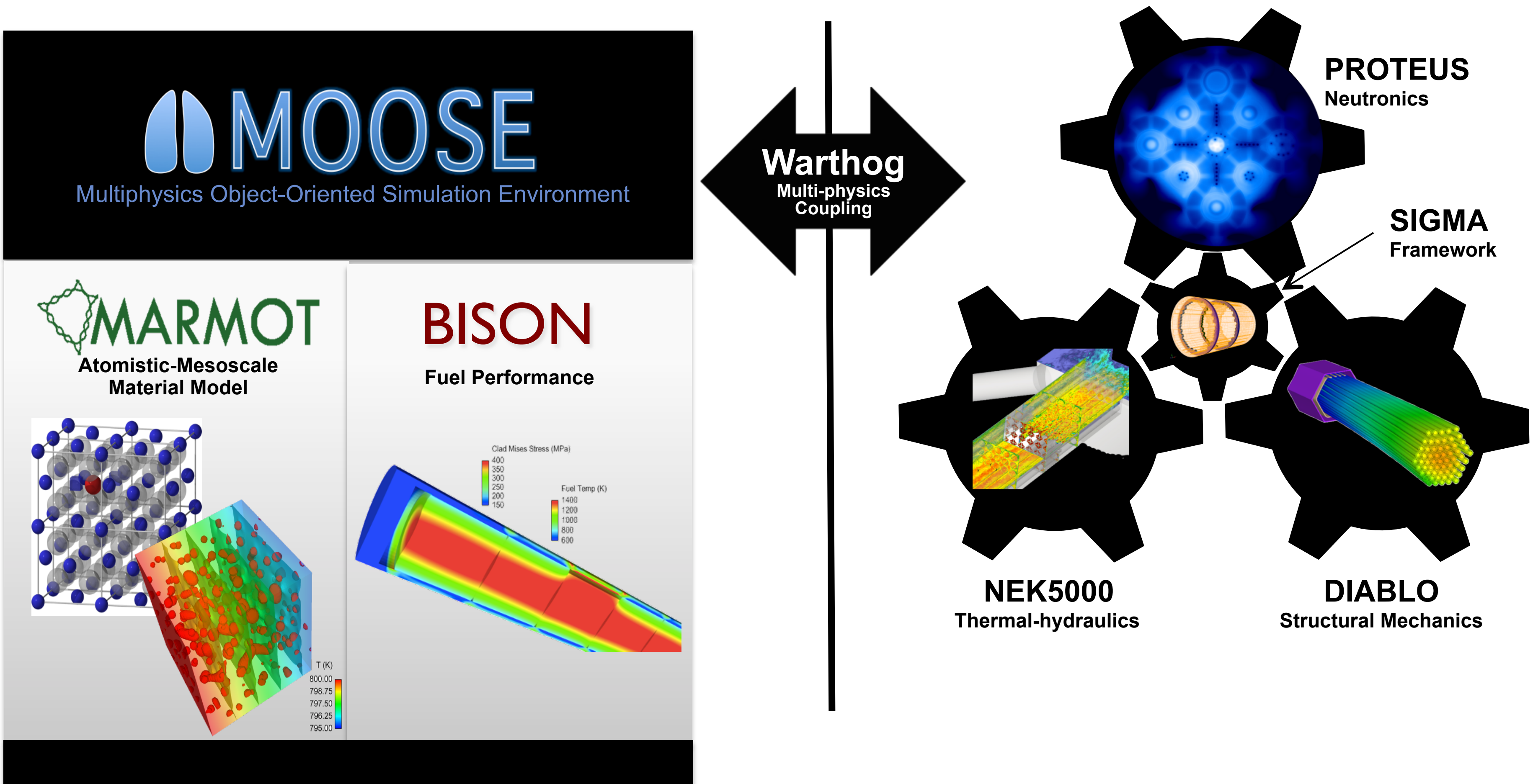
NEAMS – IPL

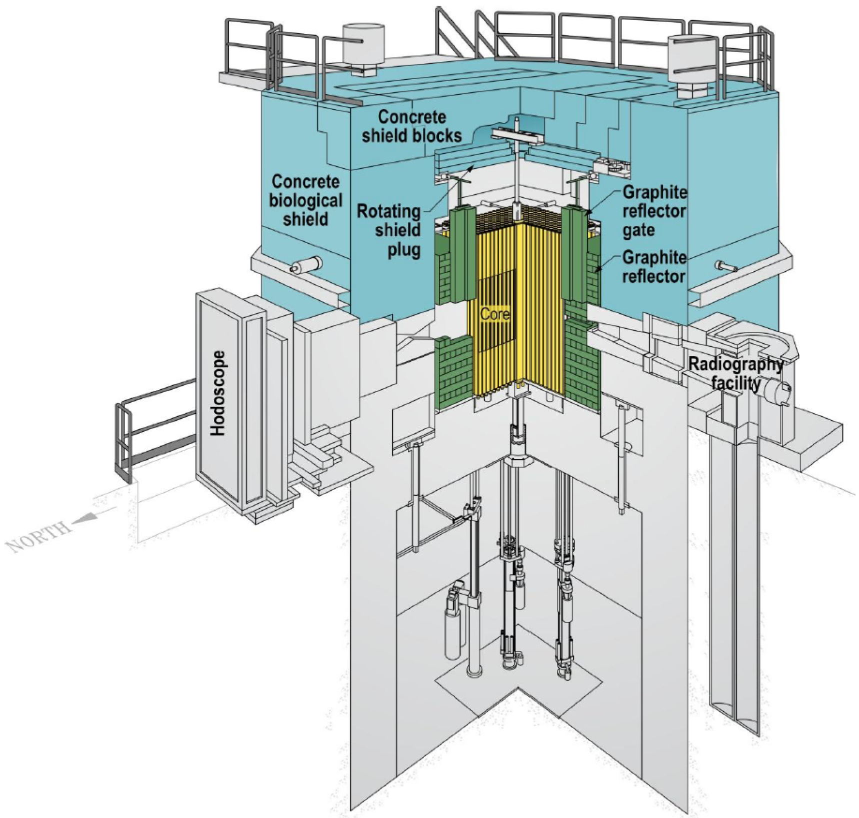
Bridging the gap between two unique frameworks to extend multi-physics coupling with advanced tools



IPL

NEAMS Support of TREAT

NE Mission Need – *Support resumption of high power/short duration transient testing at the INL TREAT facility with advanced computational tools that will enhance R&D capabilities*

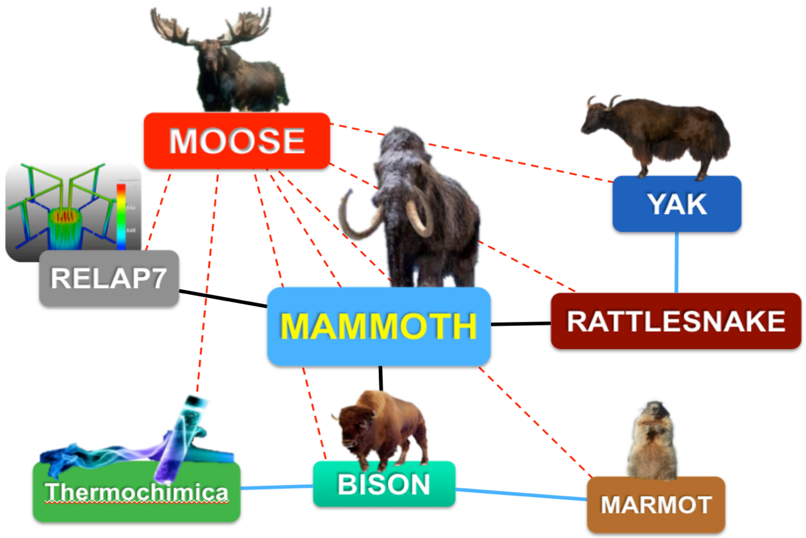


Require high-resolution reactor physics models (eventually coupled to fuel performance for irradiated fuel) to assist operation (e.g. reduce the number of calibration tests) and provide improved predictive capability for analysis of TREAT experiments.

IPL

NEAMS - Modeling TREAT Experiments

- **Primary interest is the multi-physics coupling of the core physics and the fuel experiment:**
  - core behavior with low resolution low order operator (diffusion)
    - Preferred as fastest solution
  - and experiment with high resolution high order operator (S_N)
    - Preferred as most detailed solution in smaller experiment.
- **But, in order to have the necessary flexibility for experiment design and analysis, a 3-D M&S capability is necessary to accurately predict:**
  - rapid transient behavior with detailed non-linear temperature feedback effects, and
  - high-resolution flux, fluence, power, temperature distributions and fluid states in the experiment.



NEAMS – High-Impact Problems

- **A HIP is a collaborative 3-year project that will significantly improve an application of exceptional importance for the customer through use and validation of NEAMS tools**
  - **Demonstrate efficacy** of NEAMS tools, and support their **validation** in well-defined applications, which is critical to their **deployment** (especially to industry), **utility**, and **long-term value**

- **Two High-Impact Problems started in FY 2015**
  - Accident Tolerant Fuels (ATF) - *NE Advanced Fuels Campaign*
    - Develop simulation capability to evaluate leading ATF material concepts for eventual down selection; permit use of standardized technical metrics, and provide material behavior insights that allow a quantitative basis for evaluation
  - Steam Generator Flow-Induced Vibration (SG FIV) - *NuScale Power and Areva, Inc.*
    - Develop simulation capability to assess flow induced vibration and optimize advanced steam generator designs (to be safer, more reliable); provide FIV/fluid elastic instability insights that will reduce development time and testing costs

NEAMS – NEUP/CINR
Work-scope Description

- **Program Support in Science & Technology Innovation – NEAMS-1; we are seeking proposals that contribute to improving the mechanistic models, computational methods, validation basis, and code integration and deployment for the NEAMS tools and their components in following six topical areas:**
  - NEAMS 1.1 – Atomistic and Mesoscale Modeling and Simulation of Nuclear Fuels, Cladding, and Reactor Structural Materials
  - NEAMS 1.2 – Macroscale Fuel Performance
  - NEAMS 1.3 – Core Neutronics
  - NEAMS 1.4 – Thermal Hydraulics
  - NEAMS 1.5 – Structural Mechanics
  - NEAMS 1.6 – Integration and Demonstration

NEAMS – NEUP/CINR
Work-scope Description

- **NEAMS 1.1 – Atomistic and Mesoscale Modeling and Simulation of Nuclear Fuels, Cladding, and Reactor Structural Materials**
  - Proposals are sought which improve predictive capabilities for additional phenomena of interest in nuclear materials impacting their in-reactor performance;
  - Extend the capabilities of MARMOT to a broader range of fuel and cladding materials; and
  - Improve the validation basis of the code.
  - Examples of additional phenomena of interest include corrosion, creep, chemical interaction, and phase separation in multi-phase, multi-component systems in reactor materials including current and future reactors.
  - Validation should involve closely correlated experiments and modeling using MARMOT, as well as uncertainty quantification.
  - Proposals on atomistic to mesoscale and physics coupling using MARMOTare also encouraged.
- **NEAMS 1.2 – Macroscale Fuel Performance**
  - Proposals are sought that aid in the development of theory-based models of advanced materials' properties;
  - Offer more robust and efficient numerical algorithms;
  - Extend capabilities of BISON to fuel forms that are currently under supported or not supported; and
  - Improve the validation basis of BISON, particularly for 3-D problems.
  - Proposals that employ coupling of BISON and MARMOT simulations using hierarchical, concurrent, or hybrid approaches are encouraged.

NEAMS – NEUP/CINR
Work-scope Description

NEAMS 1.3 – Core Neutronics

- Proposals are sought to improve solution accuracy, computational performance and efficiency, and verification and validation of MC2-3 for various fast and thermal reactor applications, by introducing Monte Carlo approaches, coherent coupling with PROTEUS, efficient parallelization and numerical algorithms, and advanced uncertainty evaluation techniques.

NEAMS 1.4 – Thermal Hydraulics

- Proposals are sought that develop and implement advanced turbulence models for turbulent heat fluxes in liquid metal fuel assemblies within Nek5000.
- Priority will be given to proposals that cover unsteady approaches (URANS and Hybrid LES-RANS) in both forced and natural convection.
- The models should be developed with particular attention to verification/validation using existing experimental or DNS data. Proposals that include development of new tailored DNS datasets are also encouraged.

NEAMS – NEUP/CINR
Work-scope Description

NEAMS 1.5 – Structural Mechanics

- Proposals are sought which add models to Diablo to enhance its ability to predict the thermo-mechanical response of fast reactor fuel assemblies;
- Provide more advanced, higher-fidelity approaches to resolve the inter-duct contact forces and the cross-sectional distortion effect of each duct (e.g., by representing fuel assemblies as thin shell structures), in order to more accurately calculate the core distortion and the mechanical behavior of fast reactors.
- In order to more accurately capture the cross-sectional distortion of hexagonally shaped fuel assembly ducts by contact loads (not only the displacement of an actual contact surface but also the consequent interaction among hexagonal duct walls), new models are needed in in DIABLO to simulate thermal expansion and irradiation-induced swelling and creep of the fuel assembly ducts.

NEAMS 1.6 – Integration and Demonstration

- Proposals are sought to integrate high-fidelity as well as conventional tools into the Workbench;
- Automate analysis workflows used in design studies;
- Provide convenient access to uncertainty quantification; and
- Develop and demonstrate templates of complex system models, provide automated meshing, and demonstrate the use of the Workbench for practical studies.
- Proposals that demonstrate the value of the high-fidelity NEAMS tools as applied to collaborative benchmarks, validation, and industrial systems as well as the use of NEAMS tools to inform the improved use of conventional tools within the Workbench are strongly encouraged.

NEAMS – NEUP/CINR
Work-scope Description

- **Collaboration with members of the NEAMS development team residing at DOE laboratories as well as end users in industry or regulatory authorities is strongly encouraged.**

- **Running simulations or conducting experiments at DOE laboratories or and Nuclear Science User Facilities (http://atrnsuf.inl.gov/) in support of the NEAMS Toolkit are encouraged, although computation or experimentation at university laboratories is equally acceptable.**

- **Please focus your application, if possible, on one of the six scope areas**

- **POCs**
  - Federal – Dan Funk (dan.funk@hq.doe.gov; 301-903-3845)
  - Technical – Brad Rearden (reardenb@ornl.gov; 865-574-6085)